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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/077,036	02/15/2002	Michael Andrew Parker	SJO919990205US1	1965

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EXAMINER

JOHNSTON, PHILLIP A

ART UNIT	PAPER NUMBER
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2881

DATE MAILED: 05/27/2003

Please find below and/or attached an Office communication concerning this application or proceeding.

Office Action Summary

Application No.

10/077,036

Applicant(s)

PARKER ET AL.

Examiner

Phillip A Johnston

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-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133).
- Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) ☐ Responsive to communication(s) filed on ____.
- 2a) ☐ This action is **FINAL**. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) ☒ Claim(s) 1-69 is/are pending in the application.
- 4a) Of the above claim(s) ____ is/are withdrawn from consideration.
- 5) ☐ Claim(s) ____ is/are allowed.
- 6) ☒ Claim(s) 1-69 is/are rejected.
- 7) ☐ Claim(s) ____ is/are objected to.
- 8) ☐ Claim(s) ____ are subject to restriction and/or election requirement.

Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☒ The drawing(s) filed on 5/12/02 ~~45 February 2002~~ is/are: a) ☒ accepted or b) ☐ objected to by the Examiner.
- Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
- 11) ☐ The proposed drawing correction filed on ____ is: a) ☐ approved b) ☐ disapproved by the Examiner.
- If approved, corrected drawings are required in reply to this Office action.
- 12) ☐ The oath or declaration is objected to by the Examiner.

Priority under 35 U.S.C. §§ 119 and 120

- 13) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some * c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
2. ☐ Certified copies of the priority documents have been received in Application No. ____.
3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).
- * See the attached detailed Office action for a list of the certified copies not received.
- 14) ☐ Acknowledgment is made of a claim for domestic priority under 35 U.S.C. § 119(e) (to a provisional application).
- a) ☐ The translation of the foreign language provisional application has been received.
- 15) ☐ Acknowledgment is made of a claim for domestic priority under 35 U.S.C. §§ 120 and/or 121.

Attachment(s)

- 1) ☒ Notice of References Cited (PTO-892)
- 2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
- 3) ☒ Information Disclosure Statement(s) (PTO-1449) Paper No(s) 5.
- 4) ☐ Interview Summary (PTO-413) Paper No(s) ____.
- 5) ☐ Notice of Informal Patent Application (PTO-152)
- 6) ☐ Other:

Detailed Action

Claims Rejection – 35 U.S.C. 103

1. The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which the subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

2. Claims 1-69 are rejected under 35 U.S.C. 103(a) as being unpatentable over U.S. Patent Pub. No. 2002/0059047 to Haaland, in view of Obremski, U.S. Patent No. 5,498,875, and in further view of Gupta, U.S. Patent No. 5,319,586.

Regarding Claims 1-30, Haaland (047) discloses a set of hybrid least squares multivariate spectral analysis methods in which spectral shapes of components or effects not present in the original calibration step are added in a following prediction or calibration step to improve the accuracy of the estimation of the amount of the original

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components in the sampled mixture. The hybrid method herein means a combination of an initial calibration step with subsequent analysis by an inverse multivariate analysis method. A spectral shape herein means normally the spectral shape of a non-calibrated chemical component in the sample mixture but can also mean the spectral shapes of other sources of spectral variation, including temperature drift, shifts between spectrometers, spectrometer drift, etc. The shape can be continuous, discontinuous, or even discrete points illustrative of the particular effect. See Abstract

Haaland (047) also discloses that recent advances in classical least squares (CLS) algorithms have improved the range of problems that can be addressed with the new prediction-augmented classical least-squares (PACLS) methods, see pending application Ser. No. 09/518,351. It would be desirable to achieve the best features of CLS or the new PACLS algorithm, and inverse algorithms such as the PLS or principal component regression (PCR) factor analysis PCR algorithms. The combination of CLS or PACLS and PLS or PCR (or any inverse least squares based method) for spectral analysis is the subject of this invention. By combining the explicit/implicit (hard/soft) modeling of CLS and inverse methods (e.g., PLS or PCR), the best features of each method can be realized in a single hybrid method of spectral analysis. Although the discussion concentrates on a PLS application, the new hybrid method can accommodate any appropriate inverse factor analysis method. The invention also includes any multivariate calibration method that uses or contains an inverse method and allows spectral shapes (continuous or discontinuous) to be added directly

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to the method during calibration or prediction or both, such addition performed without solely weighting by a covariance matrix. See Page 2, Paragraph [0020].

Haaland (047) still further teaches that any spectral preprocessing should be applied to the original calibration spectra, the prediction spectra, and the spectral shapes added in the PACLS method. Preprocessing steps include but are not limited to baseline correction, pathlength scaling, smoothing, derivatives, normalization, variance or auto scaling, and Fourier transforms, as recited in Claim 4. When pathlength scaling is performed, pathlength adjustments are normally applied by dividing the spectra by the pathlength to compensate for the intensity variations expected for pathlength changes in the individual samples. However, this procedure scales all components of the spectra equally. Not all sources of spectral variation should have this pathlength correction applied to them. Examples of spectral variation than should not be scaled include, but are not limited to, drift of the spectrometer, spectrally active purge gas components, and spectral changes external to the sample. In order to properly handle these different spectral components, the effect of pathlength scaling can be removed from the appropriate components by scaling the non-pathlength component concentrations in the CLS calibration by the inverse of the pathlength. This procedure effectively removes the effect of inappropriate scaling of the non-pathlength spectral components.

A method to select the eigenvectors to include in the PACLS prediction from any of the analyses discussed above is based upon the use of the CLS calibration model to perform a CLS prediction on the eigenvector spectral shapes. Since the

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eigenvectors are orthogonal basis vectors, the errors from the eigenvectors are independent. Thus, the total error variance of all the spectral shapes included in the eigenvector decomposition is the sum of the error variances of the individual errors from each eigenvector. Therefore, the eigenvectors can be selected from those that represent the largest error sources in the standard CLS calibration (or PACLS calibration if spectral shapes are included during the building of the calibration model and additional shapes are to be included during true prediction or validation). See Page 5, Paragraph [0042] and [0043].

Haaland (047) as applied above does not specifically disclose the use of target factor analysis, as recited in Claim 1. However, Obremski (875) discloses that spectroscopic measurements have some uncertainty. If the predominant uncertainty is not in the spectroscopic data, then the inverse least squares method is preferred. Otherwise, the classical least squares method is preferred. The fewer matrix inversions required by the inverse least squares approach tend to outweigh the potential benefits of a change in coordinates during the regression steps. Inverse least squares is the preferred method because of greater resistance to problems with near singular matrices. The problems of matrix singularity in multiple linear regression determinations is reduced by using orthogonalization methods. This is an eigenvector analysis by singular value decomposition, or factor analysis. An orthogonal matrix is one where all the column vectors are mutually perpendicular. Orthogonalization of a matrix prior to an inverse least squares method permits inversion of the matrix without singularity problems. This technique is principal

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component regression. This technique is also known as P-matrix method, target transform factor analysis or target factor analysis.

Therefore it would have been obvious to one of ordinary skill in the art that Haaland's (824) multivariate spectral analysis method can be modified to use target factor analysis in accordance with Obremski (875), to reduce problems with matrix singularity.

Haaland (047) in view of Obremski (875), as applied above does not specifically disclose the use of Gramm-Schmidt orthogonalization, as recited in Claim 12. However, Gupta (586) discloses that Mathematical operations, consistent with the Gramm-Schmidt method of orthogonalization, can now be performed on these $n-1$ vectors. The result is that they are rotated in hyperspace so that they are orthogonal to each other and remain orthogonal to the solution vector. This operation describes the direction of the solution vector. The intersection of this directional vector with the plane originally subtracted from the other $n-1$ planes determines the unique solution. See Column 9, line28-36.

Therefore it would have been obvious to one of ordinary skill in the art that the multivariate spectral analysis method of Haaland (824) in view of Obremski (875) can be modified to use the Gramm-Schmidt orthogonalization method in accordance with Gupta(586), to further reduce problems with matrix singularity.

Regarding Claims 31-69, Haaland (047) further discloses that the hybrid methods disclosed can be used for any quantitative spectral analysis independent of the type of

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spectroscopy used. These methods can be used in any spectroscopy where the spectral data are related to the parameters of interest. In addition to quantitation, qualitative and classification analyses can be performed with the hybrid algorithms. Types of spectroscopy where these methods might be used include, but are not restricted to, 1) infrared, 2) near-infrared, 3) visible, 4) ultraviolet, 5) X-ray, 6) gamma-ray, 7) Raman, 8) mass spectroscopy, 9) ion-mobility mass spectroscopy, 10) Auger, 11) fluorescence, 12) phosphorescence, 13) ESCA, 14) far-infrared, 15) microwave, 16) x-ray fluorescence, 17) NMR, 18) energy loss spectroscopy, 19) EDAX, 20) ESR, and 21) multi- and hyper-spectral imaging. These spectroscopic methods can be used in absorption, transmission, reflection, or emission modes. In addition, the hybrid methods can be applied to other forms of multivariate data such as seismic data, chromatographic data, thermal gravimetric analysis, and image data. The hybrid algorithm can also be used for outlier or anomaly detection by examining various outlier metrics such as Mahalanobis distance, spectral residuals, spectral F ratios, or other statistical indications of spectra that lie outside the hybrid model. This additional capability is ideally suited for multi- and hyperspectral image analysis. With the outlier metrics obtained from hybrid algorithm, the hybrid method can also be used for classification purposes. In this discussion, spectral components can include either chemical components (molecular or elemental) or other sources of spectral change that include but are not limited to spectrometer/system drift, chromatic aberrations, diffraction effects, temperature changes, sample insertion and alignment effects, purge

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changes, alignment changes, detector changes and nonlinearities, source changes, and changes in spectrometer components to include even substitution of whole spectrometers. See Page 5, Paragraph[0027].

Conclusion

3. Any inquiry concerning this communication or earlier communications should be directed to Phillip Johnston whose telephone number is (703) 305-7022. The examiner can normally be reached on Monday-Friday from 7:30 am to 4:00 pm. If attempts to reach the examiner by telephone are unsuccessful, the examiners supervisor John Lee can be reached at (703) 308-4116. The fax phone numbers are (703) 872-9318 for regular response activity, and (703) 872-9319 for after-final responses. In addition the customer service fax number is (703) 872- 9317.

Any inquiry of a general nature or relating to the status of this application or proceeding should be directed to the receptionist whose telephone number is 703 308 0956.

PJ
May 16, 2003


JOHN R. LEE
SUPERVISORY PATENT EXAMINER
TECHNOLOGY CENTER 2800